Supporting Information

Defects and Dopants in $CaFeSi_2O_6$: A combined classical and DFT simulation

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Table S1. Interatomic potential parameters used in the atomistic simulations of $CaFeSi_2O_6$.

Two-body [$\Phi_{ij}(r_{ij}) = A_{ij}\exp(-r_{ij}/\rho_{ij}) - C_{ij}/r_{ij}^6$]

Interaction	A / eV	ρ / Å	C / eV·Å^6	Y / e	K / eV·Å^{-2}
Ca^{2+}–O^{2-}(1)	1090.40	0.3372	0.0000	1.26000	34.00
Fe^{2+} - O^{2-}(2)	1105.2409	0.3106	0.0000	2.99700	19.26
O^{2-}–O^{2-}(3)	22764.30	0.1490	27.879	–2.860	74.92
Si^{4+} - O^{2-}(3)	1283.91	0.32052	10.66	4.000	99999
Sr^{2+} - O^{2-}(1)	1400.00	0.3500	0.0000	0.6700	21.53
Ba^{2+} - O^{2-}(1)	931.79	0.3949	0.0000	0.5400	14.78
Co^{2+} - O^{2-}(1)	696.3	0.3362	0.0000	2.000	10.74
Ni^{2+} - O^{2-}(1)	683.5	0.3332	0.0000	2.000	8.77
Zn^{2+} - O^{2-}(1)	499.60	0.3595	0.0000	2.050	10.28
Mg^{2+} - O^{2-}(4)	946.627	0.31813	0.0000	2.000	99999
Mn^{2+} - O^{2-}(3)	2601.394	0.2780	0.0000	3.420	95.0
Al^{3+} - O^{2-}(5)	1725.20	0.28971	0.0000	3.000	99999
Ga^{3+} - O^{2-}(4)	2901.12	0.2742	0.0000	3.000	99999
Sc^{3+} - O^{2-}(1)	1299.40	0.3312	0.0000	3.000	99999
In^{3+} - O^{2-}(6)	1495.65	0.3327	0.0000	3.000	99999
Y^{3+} - O^{2-}(7)	1345.10	0.3491	0.0000	3.000	99999
Gd^{3+} - O^{2-}(8)	1885.75	0.3399	20.34	3.000	99999
La^{3+} - O^{2-}(9)	1545.21	0.3590	0.000	–0.250	145.0
Ge^{4+} - O^{2-}(6)	1497.3996	0.325646	16.00	4.000	99999
Sn^{4+} - O^{2-}(7)	1414.32	0.3479	13.660	4.000	99999
Ti^{4+} - O^{2-}(12)	5111.7	0.2625	0.0000	–0.10	314.0
Zr^{4+} - O^{2-}(11)	1502.11	0.3477	5.10	1.65	189.70
Ce^{4+} - O^{2-}(1)	1986.83	0.3511	20.40	7.700	291.75

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